

Extended Cut Method for Edge Wiener, Schultz and Gutman Indices with Applications

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Abstract

A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. In this paper we extend the well known cut method to certain distance and degree based topological indices such as edge Wiener, Schultz and Gutman indices. As applications, we compute these indices for regular and irregular convex triangular hexagon.

1 Introduction

Throughout the paper, we consider simple and finite graph G with vertex set $V(G)$ and edge set $E(G)$. A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A molecular graph is a collection of vertices

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representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry.

The line graph $L(G)$ of a graph G is a graph with vertex set as $E(G)$ and two vertices of $L(G)$ are adjacent if and only if they have a common vertex in G . For two vertices $u, v \in V(G)$, the distance $d_G(u, v)$ is defined as the length of a shortest path connecting u and v in G . Similarly, for any two edges $f = (a, b)$ and $g = (u, v)$ in $E(G)$, the distance $D_G(f, g)$ is defined as $\min\{d_e(a, g), d_e(b, g)\}$ where $d_e(a, g) = \min\{d_G(a, u), d_G(a, v)\}$ and $d_e(b, g)$ is defined analogously. Clearly, $D_G(f, g) = d_{L(G)}(f, g) - 1$.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. There are many examples of such graph invariants, particularly, distance and degree based which are great importance in chemical sciences. A lot of research on distance based graph invariant namely Wiener index [39] from theoretical and practical point of view [11, 12, 31] which is the sum of distances between all pairs of vertices of the molecular graph. In other words, for any connected graph G , Wiener index $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$. The edge Wiener index [7] of a G is defined as

$$W_e(G) = \sum_{\{f,g\} \subseteq E(G)} D_G(f, g) .$$

The edge Wiener index is a more interesting graph invariant and well studied by many researchers. We encourage the readers to refer the recent survey [22] for more details. In 1989, Schultz [37] introduced a graph-theoretical descriptor for characterizing alkanes by an integer namely the Schultz index and defined as

$$S(G) = \sum_{\{x,y\} \subseteq V(G)} \{\deg_G(x) + \deg_G(y)\} d_G(x, y)$$

where $\deg_G(x)$ is the degree of vertex x in G and $\deg_G(y)$ is defined analogously. The Schultz index attracted much attention after it was discovered [10, 16, 27, 29] and it has been shown that $S(G)$ and $W(G)$ are closely mutually related for certain classes of molecular graphs. In particular, for any tree T of order n , there is an explicit relation that $S(T) = 4W(T) - n(n - 1)$.

The Gutman index [16], a Schultz-type molecular topological index is a natural extension of the Wiener index. The Gutman index of a graph G is defined as

$$Gut(G) = \sum_{\{x,y\} \subseteq V(G)} \deg_G(x) \deg_G(y) d_G(x, y) .$$

For acyclic structures, the Gutman index is closely related to the Wiener index and reflects precisely the same structural features of a molecular as the Wiener index [16]. The theoretical investigations of Gutman index focusing on polycyclic structures have attracted many researchers [1–3, 6, 13] and the upper bound on Gutman index of graphs have been discussed in many papers [3, 7, 14, 35, 36].

The rest of the paper is organized as follows: In Section 2, we discuss the popular cut method on topological indices and extend it for well recognized indices such as edge Wiener index, Schultz index and Gutman index. We compute these indices for hexagonal network and irregular convex triangular hexagon in Section 3. Finally, in Section 4, we conclude the paper with a remark.

2 Extended cut method

We begin this section by introducing a few basic concepts on cut method. A subgraph H of a graph G is convex if for any vertices $u, v \in V(H)$, any shortest path in G between u and v lies completely in H . On the other side, H is called an isometric subgraph of G if $d_H(u, v) = d_G(u, v)$. Clearly, a convex subgraph is isometric but not the other way around.

The hypercube of dimension n , denoted by Q_n , $n \geq 1$, is the Cartesian product of n copies of the complete graph K_2 . In other words, if we set $V(K_2) = \{0, 1\}$, then the vertex set of Q_n consists of all binary strings of length n over $\{0, 1\}$ and two such strings are adjacent if and only if they differ in exactly one position. Let G be connected graph, then G is called a partial cube if its vertices can be labeled with binary strings of a fixed length such that $d_G(u, v) = H(l(u), l(v))$ holds for any two vertices u and v of G with labels $l(u)$ and $l(v)$ respectively, where $H(l(u), l(v))$ is the Hamming distance between the binary strings $l(u)$ and $l(v)$. The edges $e = (x, y)$ and $f = (u, v)$ of G are in the Djoković-Winkler [9, 40] relation Θ if $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$. The relation is always reflexive and symmetric, and is transitive on partial cubes. Then the relation Θ partitions the edge set of a partial cube G into Θ -classes F_1, F_2, \dots, F_k , where e and f lie in a common class F_i if and only if $e \Theta f$. Moreover, for any index i , the graph $G - F_i$ consists of exactly two connected components [40].

The cut method is a powerful tool for the investigation of distance and degree based molecular structure-descriptors (also called topological indices). These indices are used in

theoretical chemistry for the design of quantitative structure-property relations (QSPR) and quantitative structure-activity relations (QSAR). For more details on cut method, we refer to the recent survey [31]. For completeness, we give the general form of cut method as follows.

If G is a molecular graph, then (i) partition the edge set of G into classes F_1, F_2, \dots, F_k , called cuts, such that each of the graphs $G - F_i$, $1 \leq i \leq k$, consists of at least two connected components; and then (ii) use properties of the components of the graphs $G - F_i$ to derive a required property of G [26].

The first application of the cut method is the following theorem. For another aspect and application of the theorem found in [17, 19].

Theorem 2.1. [28] *Let G be a partial cube and let F_1, F_2, \dots, F_k be its Θ -classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Then $W(G) = \sum_{i=1}^k n_1(F_i) n_2(F_i)$.*

The above Theorem was applied in several papers to obtain closed expressions for the Wiener index of chemical graphs and also the cut method was successively applied to compute vertex-Szeged index [18], edge Wiener and edge-Szeged indices [41], total-Szeged index [34], PI index [23, 25], generalized terminal Wiener index [20], Gutman and Schultz indices [24]. Hence the cut method is found efficient in the families of partial cube. Cut method that apply to classes larger than partial cubes will be called extended cut method. We need the following concepts for the further study.

A graph G is an l_1 -graph if it admits a scale λ embeddable into a hypercube, where a scale λ embeddable of H into G is a mapping $\iota : V(H) \rightarrow V(G)$ such that $d_G(\iota(u), \iota(v)) = \lambda d_H(u, v)$ holds for some fixed integer λ and all vertices $u, v \in V(H)$.

Suppose that F is a cut of G such that $G - F$ consists of two components, say, GF^1 and GF^2 . Then F is called a convex cut if both GF^1 and GF^2 are convex subgraphs of G . Let $E^\lambda(G)$, $\lambda \geq 1$, denote a collection of edges of a graph G with each edge in G is repeated exactly λ times. It was well noted that a graph G admits a partition of $E^\lambda(G)$ into convex cuts if and only if G is a l_1 -graph [8]. Moreover, it was observed for $\lambda = 1$ in [30].

The first extension of the cut method appeared in [5] for computing Wiener index of families of l_1 -graph and stated as follows.

Theorem 2.2. [5] *Let G be a scale λ embeddable into a hypercube and let $\mathcal{C}(G)$ be the family of convex cuts of $E^\lambda(G)$ defining this embedding. Then $W(G) = \frac{1}{\lambda} \sum_{F \in \mathcal{C}(G)} |V(GF^1)| |V(GF^2)|$.*

In the bipartite case, l_1 -graphs coincide with partial cubes, hence their generalization is important in the non-bipartite case which indeed contains many chemical graphs [31]. We now extend the cut method to compute edge Wiener, Schultz and Gutman indices of l_1 -graphs. First, we outline the proof of cut method on these indices with respect to partial cubes.

Lemma 2.3. [24] *A connected graph G admits a partition $\{F_i\}_{i=1}^r$ of $E(G)$ into convex cuts with components GF_i^1 and GF_i^2 for each i . Let R be a set of shortest paths with the property that for each pair of vertices of G there exists a unique path in R connecting them. For any $P_G(u, v) \in R$ and each i , the following statements hold:*

- (i) If $\{u, v\} \subseteq V(GF_i^1)$ or $\{u, v\} \subseteq V(GF_i^2)$, then $|E(P_G(u, v)) \cap F_i| = 0$,
- (ii) If $u \in V(GF_i^1)$ and $v \in V(GF_i^2)$, then $|E(P_G(u, v)) \cap F_i| = 1$.

Lemma 2.4. [41] *A connected graph G admits a partition $\{F_i\}_{i=1}^r$ of $E(G)$ into convex cuts with components GF_i^1 and GF_i^2 for each i . Let S be a set of shortest paths with the property that for each pair of edges of G there exists a unique path in S connecting them. For any $P_G(e, f) \in S$ and each i , the following statements hold:*

- (i) If $\{e, f\} \subseteq E(GF_i^1)$, $\{e, f\} \subseteq E(GF_i^2)$ or $\{e, f\} \subseteq F_i$, then $|E(P_G(e, f)) \cap F_i| = 0$,
- (ii) If $e \in F_i$ and $\{f \in E(GF_i^1)$ or $f \in E(GF_i^2)\}$, then $|E(P_G(e, f)) \cap F_i| = 0$,
- (iii) If $e \in E(GF_i^1)$ and $f \in E(GF_i^2)$, then $|E(P_G(e, f)) \cap F_i| = 1$.

Remark: Lemmas 2.3 and 2.4 are valid when G admits a partition $\{F_i\}_{i=1}^m$ of $E^\lambda(G)$ into convex cuts.

Theorem 2.5. [24, 41] *A connected graph G admits a partition $\{F_i\}_{i=1}^r$ of $E(G)$ into convex cuts with components GF_i^1 and GF_i^2 for each i . Then*

- (i) $W_e(G) = \sum_{i=1}^r |E(GF_i^1)| |E(GF_i^2)|$,

(ii) $S(G) = |E(G)| |V(G)| + 2 \sum_{i=1}^r (|V(GF_i^1)| |E(GF_i^2)| + |V(GF_i^2)| |E(GF_i^1)|),$

(iii) $Gut(G) = 2 |E(G)|^2 + \sum_{i=1}^r (4 |E(GF_i^1)| |E(GF_i^2)| - |F_i|^2).$

As a consequence of above theorem, we have the following result.

Theorem 2.6. *A connected graph G admits a partition $\{F_i\}_{i=1}^m$ of $E^\lambda(G)$ into convex cuts with components GF_i^1 and GF_i^2 for each i . Then*

(i) $W_e(G) = \frac{1}{\lambda} \sum_{i=1}^m |E(GF_i^1)| |E(GF_i^2)|,$

(ii) $S(G) = |E(G)| |V(G)| + \frac{2}{\lambda} \sum_{i=1}^m (|V(GF_i^1)| |E(GF_i^2)| + |V(GF_i^2)| |E(GF_i^1)|),$

(iii) $Gut(G) = 2 |E(G)|^2 + \frac{1}{\lambda} \sum_{i=1}^m (4 |E(GF_i^1)| |E(GF_i^2)| - |F_i|^2).$

Proof. Let S be a set of shortest paths between pairs of edges of G such that for each edge $f, g \in E(G)$ there is a unique shortest path $P_G(f, g)$ connecting them. For any edge $h \in E(G)$, define $\eta_S(h) = |\{P_G(f, g) \in S : h \in E(P_G(f, g))\}|$. Then $W_e(G) = \frac{1}{\lambda} \sum_{h \in E(G)} \eta_S(h) = \frac{1}{\lambda} \sum_{i=1}^m |E(GF_i^1)| |E(GF_i^2)|.$

Let R be a set of shortest paths between pairs of vertices of G such that for each vertex $u, v \in V(G)$ there is a unique shortest path $P_G(u, v)$ connecting them. Suppose there are k paths $P_G(u_1, v_1), P_G(u_2, v_2), \dots, P_G(u_k, v_k)$ in R containing the edge e . Define $\eta_R(e) = \sum_{i=1}^k \{\deg_G(u_i) + \deg_G(v_i)\}$. Then $S(G) = \frac{1}{\lambda} \sum_{i=1}^m \sum_{e \in F_i} \eta_R(e) = \frac{1}{\lambda} \sum_{i=1}^m \sum_{u \in V(GF_i^1)} \sum_{v \in V(GF_i^2)} \{\deg_G(u) + \deg_G(v)\}$. Using the fact that $\sum_{u \in V(GF_i^1)} \deg_G(u) = 2 |E(GF_i^1)| + |F_i|$ and $\sum_{v \in V(GF_i^2)} \deg_G(v) = 2 |E(GF_i^2)| + |F_i|$, we get $S(G) = |E(G)| |V(G)| + \frac{2}{\lambda} \sum_{i=1}^m (|V(GF_i^1)| |E(GF_i^2)| + |V(GF_i^2)| |E(GF_i^1)|)$. By similar argument, $Gut(G) = 2 |E(G)|^2 + \frac{1}{\lambda} \sum_{i=1}^m (4 |E(GF_i^1)| |E(GF_i^2)| - |F_i|^2).$

3 Triangular nets

Let G be a plane graph. The boundary of G is the boundary of the unbounded face of G . The graph G is called a homogeneous n -gonal net if each bounded face of G is a regular n -side polygon. We restrict our study to homogeneous 3-gonal nets, which we call as triangular nets. Suppose $\{H_1, H_2, \dots, H_h\}$, $\{R_1, R_2, \dots, R_r\}$ and $\{L_1, L_2, \dots, L_l\}$ are three

sets of parallel lines lying on the same plane, where $h, r, l \geq 2$. Moreover the following conditions are satisfied:

- (a) All H -lines run horizontally (East–West). All R -lines run towards North–East (or South–West) cutting an H -line at an angle of $2\pi/3$. All L -lines run towards North–West (or South–East) cutting an H -line at an angle of $2\pi/3$.
- (b) Two successive lines in the same set have unit distance between them when measured along another sets of lines.
- (c) Each line has at least one point which is the intersection of three lines (called triple intersection point).

From the sets of lines $\{H_1, H_2, \dots, H_h\}$, $\{R_1, R_2, \dots, R_r\}$ and $\{L_1, L_2, \dots, L_l\}$, a graph is obtained by taking all triple intersection points as vertices and all unit line-segments joining two triple intersection points as edges. This graph is called a convex triangulation mesh, and is denoted by $\Delta_{h,r,l}$. Note that there are non-isomorphic convex triangulation meshes having the same parameters [32]. To determine a unique graph for $\Delta_{h,r,l}$, we introduce the following notations.

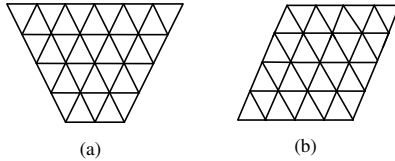


Figure 1: (a) Triangular trapezium $T_{4,6}$ (b) Triangular parallelogram $P_{4,4}$

A convex triangulation mesh $\Delta_{h,r,l}$ is called a triangular trapezium if its boundary forms a trapezium. In this case, $r = l$ and the length of the longer base and the height are $r - 1$ and $h - 1$ respectively. We denote this triangular trapezium by $T_{h-1,r-1}$. When $h = r$, $T_{h-1,r-1}$ becomes a triangular triangle which is denoted by T_{h-1} . For $n \geq 1$, $T_{1,n}$ is called a $(2n - 1)$ -triangular chain and is denoted by I_{2n-1} . $\Delta_{h,r,l}$ is called a triangular parallelogram if its boundary forms a parallelogram. In this case, $|r - l| = h - 1$ and $\Delta_{h,r,l}$ is isomorphic to $\Delta_{h,l,r}$. In the following, we shall always assume that $l > r$ and denote the triangular parallelogram $\Delta_{h,r,h+r-1}$ by $P_{h-1,r-1}$. See Figure 1. For $n \geq 1$, $P_{1,n}$ is called a $2n$ -triangular chain and denoted by I_{2n} .

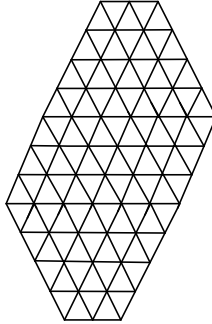


Figure 2: Irregular convex triangular hexagon $H_{4,4,3,6}$

A graph obtained by merging the longer base of $T_{p,n}$ and $T_{q,n}$ with two bases of $P_{m,n}$ forming a convex six sided polygon is called an irregular convex triangular hexagon and denoted by $H_{q,p,m,n}$ where $0 \leq p, q \leq n$ and $m \geq 0$. By reflection, $H_{q,p,m,n} \cong H_{p,q,m,n}$ and we always assume that $q \geq p$ [38]. See Figure 2. It is interesting to note that $H_{q,0,0,n} = T_{q,n} \cong T_{n,q}$, $H_{n,0,0,n} = T_n$, $H_{0,0,m,n} = P_{m,n} \cong P_{n,m}$, $H_{1,0,0,n} = I_{2n-1}$ and $H_{0,0,1,n} = I_{2n}$.

Hexagonal network is based on the partition of a plane into equilateral triangles. Hexagonal network of dimension n is denoted by $HX(n)$ and also n is the number of vertices on one side of the hexagon [4]. It has been studied in a variety of contexts [15,33]. We note that $H_{n-1,n-1,0,2(n-1)} \cong HX(n)$. See Figure 3.

In what follows, $G = H_{q,p,m,n}$. Then the number vertices and edges of G are $(n+1)(m+p+q+1) - \frac{1}{2}\{p(p+1) + q(q+1)\}$ and $m+n+3n(m+p+q) - \frac{1}{2}\{3(p^2+q^2) - (p+q)\}$ respectively. The Wiener index of $H_{q,p,m,n}$ obtained in [38] by introducing the generalized elementary cut method [Theorem 2.2 with $\lambda = 2$] of a homogeneous polygonal net. We now obtain the edge Wiener, Schultz and Gutman indices of $H_{q,p,m,n}$ using Theorem 2.6.

We partition $E^2(G)$ into three subsets $E_H(G)$, $E_R(G)$ and $E_L(G)$, which are the sets of convex cuts whose cutlines are parallel to the H -lines, R -lines and L -lines respectively. We now consider three cases.

Case A: $W_e(G) = \frac{1}{2}\{g_H + g_R + g_L\}$ where g_H , g_R and g_L are computed in the following.

We compute g_H by considering the bottom layer as the first layer, let F_i , $1 \leq i \leq m+p+q$, be the convex cut of G , which passes through the i^{th} layer of G (edges between i^{th} and $(i+1)^{\text{th}}$ H-lines).

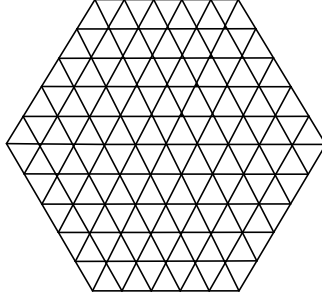


Figure 3: Hexagonal network $HX(6)$

$$\text{We have } |F_i| = \begin{cases} 2(n-q+i) & : & 1 \leq i \leq q \\ 2n+1 & : & q < i \leq m+q \\ 2(m+q+n+1-i) & : & m+q < i \leq m+p+q, \end{cases}$$

$$|V(GF_i^1)| = \begin{cases} \sum_{j=1}^i (n-q+j) & : & 1 \leq i \leq q \\ \sum_{j=1}^{q+1} (n-q+j) + (i-q-1)(n+1) & : & q < i \leq m+q \\ |V(G)| - \sum_{j=1}^{m+p+q+1-i} (n-p+j) & : & m+q < i \leq m+p+q, \end{cases}$$

$$|E(GF_i^1)| = \begin{cases} 3 \sum_{j=1}^i (n-q+j-1) - 2(n-q) & : & 1 \leq i \leq q \\ 3 \sum_{j=1}^{q+1} (n-q+j-1) - 2(n-q) + (i-q-1)(3n+1) & : & q < i \leq m+q \\ |E(G)| - 3 \sum_{j=1}^{m+p+q+1-i} (n-p+j-1) + 2(n-p) - 2(m+q+n+1-i) & : & m+q < i \leq m+p+q. \end{cases}$$

Hence $g_H = \sum_{i=1}^{m+p+q} |E(GF_i^1)| \{ |E(G)| - |E(GF_i^1)| - |F_i| \} = g(q, p, m, n)$, say.

Similar expression may be obtained for g_R and g_L after rotating G for $2\pi/3$ and $4\pi/3$ radians in clock-wise respectively [38]. Therefore,

$$g_R = \begin{cases} g(m+q, m+p, n-m-q-p, m+q+p) & : & q+p \leq n-m \\ g(n-p, n-q, m+q+p-n, n) & : & q+p \geq n-m, \end{cases}$$

$$g_L = \begin{cases} g(q, p, n-q-p, m+q+p) & : & q+p \leq n \\ g(n-p, n-q, q+p-n, m+n) & : & q+p \geq n. \end{cases}$$

Case B: $S(G) = |E(G)| |V(G)| + \{s_H + s_R + s_L\}$ where

$$s_H = \sum_{i=1}^{m+p+q} |V(GF_i^1)| \{|E(G)| - |E(GF_i^1)| - |F_i|\} + |E(GF_i^1)| \{|V(G)| - |V(GF_i^1)|\} = s(q, p, m, n), \text{ say.}$$

$$s_R = \begin{cases} s(m+q, m+p, n-m-q-p, m+q+p) & : q+p \leq n-m \\ s(n-p, n-q, m+q+p-n, n) & : q+p \geq n-m, \end{cases}$$

$$s_L = \begin{cases} s(q, p, n-q-p, m+q+p) & : q+p \leq n \\ s(n-p, n-q, q+p-n, m+n) & : q+p \geq n. \end{cases}$$

Case C: $Gut(G) = 2|E(G)|^2 + \frac{1}{2}\{t_H + t_R + t_L\}$ where

$$t_H = \sum_{i=1}^{m+p+q} 4|E(GF_i^1)| \{|E(G)| - |E(GF_i^1)| - |F_i|\} - |F_i|^2 = t(q, p, m, n), \text{ say.}$$

$$t_R = \begin{cases} t(m+q, m+p, n-m-q-p, m+q+p) & : q+p \leq n-m \\ t(n-p, n-q, m+q+p-n, n) & : q+p \geq n-m, \end{cases}$$

$$t_L = \begin{cases} t(q, p, n-q-p, m+q+p) & : q+p \leq n \\ t(n-p, n-q, q+p-n, m+n) & : q+p \geq n. \end{cases}$$

After some computation by MATLAB software, we have the following examples.

Example 1. Let $G = H_{q,p,m,n}$ and if $q+p \leq n-m$, then

(a) $W_e(G) = -(9m^5 - 45m^4n + 45m^4p + 45m^4q - 90m^3n^2 - 180m^3np - 180m^3nq - 120m^3n + 45m^3p^2 + 180m^3pq - 15m^3p + 135m^3q^2 + 15m^3q + 15m^3 - 180m^2n^3 - 270m^2n^2p - 270m^2n^2q + 270m^2n^2 - 540m^2npq - 270m^2np - 270m^2nq + 75m^2n - 315m^2p^3 + 405m^2p^2q + 135m^2p^2 + 405m^2pq^2 - 90m^2pq + 75m^2p + 225m^2q^3 + 135m^2q^2 + 75m^2q + 60m^2 - 360mn^3p - 360mn^3q - 120mn^3 - 540mn^2pq + 630mn^2p + 630mn^2q + 180mn^2 - 540mnp^2 - 360mnpq + 30mnp - 540mnq^2 + 30mnq - 150mn - 270mp^4 - 270mp^3q + 45mp^3 + 540mp^2q^2 + 225mp^2q + 180mp^2 + 450mpq^3 + 45mpq^2 + 90mpq + 75mp + 90mq^4 + 45mq^3 - 30mq^2 + 45mq - 24m - 180n^3p^2 - 360n^3pq - 120n^3p - 180n^3q^2 - 120n^3q - 20n^3 - 90n^2p^3 + 270n^2p^2q + 540n^2p^2 + 630n^2pq + 210n^2p + 180n^2q^3 + 450n^2q^2 + 210n^2q + 60n^2 + 225np^4 - 180np^3q - 660np^3 - 135np^2q^2 - 405np^2q - 15np^2 - 495npq^2 - 225npq - 210np - 90nq^4 - 480nq^3 - 120nq^2 - 210nq - 40n - 144p^5 - 180p^4q + 195p^4 + 180p^3q^2 + 60p^3q + 50p^3 + 270p^2q^3 + 315p^2q^2 + 165p^2q + 195p^2 + 90pq^4 - 30pq^3 + 45pq^2 - 15pq + 4p + 36q^5 + 150q^4 + 20q^3 + 150q^2 + 4q)/120$

(b) $S(G) = -(6m^5 - 30m^4n + 30m^4p + 30m^4q - 60m^3n^2 - 120m^3np - 120m^3nq - 160m^3n + 30m^3p^2 + 120m^3pq - 20m^3p + 90m^3q^2 + 20m^3q - 50m^3 - 120m^2n^3 - 180m^2n^2p - 180m^2n^2q - 360m^2n^2 - 360m^2npq - 360m^2np - 360m^2nq - 330m^2n - 210m^2p^3 + 270m^2p^2q - 45m^2p^2 + 270m^2pq^2 + 60m^2pq - 105m^2p + 150m^2q^3 + 225m^2q^2 - 75m^2q - 60m^2 - 240mn^3p - 240mn^3q - 160mn^3 - 360mn^2pq - 600mn^2p - 600mn^2q - 360mn^2 -$

$$480mnpq - 420mnp - 420mnq - 220mn - 180mp^4 - 180mp^3q - 210mp^3 + 360mp^2q^2 + 120mp^2q - 15mp^2 + 300mpq^3 + 420mpq^2 - 60mpq - 55mp + 60mq^4 + 150mq^3 + 75mq^2 - 65mq - 16m - 120n^3p^2 - 240n^3pq - 160n^3p - 120n^3q^2 - 160n^3q - 40n^3 - 60n^2p^3 + 180n^2p^2q - 180n^2p^2 - 420n^2pq - 300n^2p + 120n^2q^3 - 120n^2q^2 - 300n^2q - 60n^2 + 150np^4 - 120np^3q + 20np^3 - 90np^2q^2 + 90np^2q - 30np^2 - 30npq^2 - 210npq - 160np - 60nq^4 + 80nq^3 - 160nq - 20n - 96p^5 - 120p^4q - 55p^4 + 120p^3q^2 - 100p^3q - 20p^3 + 180p^2q^3 + 195p^2q^2 + 45p^2q + 55p^2 + 60pq^4 + 140pq^3 + 15pq^2 - 55pq - 4p + 24q^5 + 20q^4 + 40q^3 + 40q^2 - 4q)/60$$

(c) $Gut(G) = -(9m^5 - 45m^4n + 45m^4p + 45m^4q - 90m^3n^2 - 180m^3np - 180m^3nq - 120m^3n + 45m^3p^2 + 180m^3pq - 15m^3p + 135m^3q^2 + 15m^3q - 5m^3 - 180m^2n^3 - 270m^2n^2p - 270m^2n^2q - 270m^2n^2 - 540m^2npq - 270m^2np - 270m^2nq - 165m^2n - 315m^2p^3 + 405m^2p^2q + 135m^2p^2 + 405m^2pq^2 - 90m^2pq + 15m^2p + 225m^2q^3 + 135m^2q^2 + 15m^2q - 360mn^3p - 360mn^3q - 120mn^3 - 540mn^2pq - 450mn^2p - 450mn^2q - 120mn^2 - 360mnpq - 270mnp - 270mnq - 90mn - 270mp^4 - 270mp^3q + 45mp^3 + 540mp^2q^2 + 225mp^2q + 240mp^2 + 450mpq^3 + 45mpq^2 - 30mpq + 15mp + 90mq^4 + 45mq^3 + 30mq^2 - 15mq - 4m - 180n^3p^2 - 360n^3pq - 120n^3p - 180n^3q^2 - 120n^3q - 20n^3 - 90n^2p^3 + 270n^2p^2q - 450n^2pq - 90n^2p + 180n^2q^3 - 90n^2q^2 - 90n^2q + 225np^4 - 180np^3q - 120np^3 - 135np^2q^2 + 135np^2q + 45np^2 + 45npq^2 - 345npq - 90np - 90nq^4 + 60nq^3 - 60nq^2 - 90nq - 10n - 144p^5 - 180p^4q + 60p^4 + 180p^3q^2 + 60p^3q + 80p^3 + 270p^2q^3 + 45p^2q^2 + 135p^2q + 90p^2 + 90pq^4 - 30pq^3 + 15pq^2 - 45pq + 4p + 36q^5 + 15q^4 + 50q^3 + 45q^2 + 4q)/30$

Example 2. Let $G = H_{q,p,m,n}$ and if $n - m \leq q + p \leq n$, then

(a) $W_\epsilon(G) = (180m^3n^2 + 120m^3n + 20m^3 + 90m^2n^3 + 540m^2n^2p + 540m^2n^2q - 270m^2n^2 - 270m^2np^2 + 270m^2np - 270m^2nq^2 + 270m^2nq - 180m^2n + 270m^2p^3 - 270m^2p^2q - 180m^2p^2 + 90m^2pq + 30m^2p - 90m^2q^2 + 30m^2q - 60m^2 + 45mn^4 + 180mn^3p + 180mn^3q + 120mn^3 + 270mn^2p^2 + 1080mn^2pq - 630mn^2p + 270mn^2q^2 - 630mn^2q - 75mn^2 - 180mnp^3 - 540mnp^2q + 540mnp^2 - 540mnpq^2 + 360mnpq - 240mnp - 180mnq^3 + 540mnq^2 - 240mnq + 150mn + 180mp^4 + 180mp^3q - 90mp^3 - 135mp^2q^2 - 225mp^2q - 30mp^2 + 45mpq^2 + 135mpq - 60mp - 45mq^4 - 90mq^3 + 75mq^2 - 60mq + 40m - 9n^5 + 45n^4p + 45n^4q + 135n^3p^2 + 180n^3pq + 135n^3p + 45n^3q^2 + 105n^3q - 15n^3 + 180n^2p^3 - 540n^2p^2 + 270n^2pq^2 - 630n^2pq - 105n^2p - 90n^2q^3 - 450n^2q^2 - 105n^2q - 60n^2 - 270np^4 + 660np^3 - 270np^2q^2 + 360np^2q - 135np^2 - 180npq^3 + 450npq^2 + 195np + 180nq^4 + 570nq^3 +$

$$75nq^2+225nq+24n+108p^5+90p^4q-210p^4-45p^3q^2-45p^3q+30p^3+45p^2q^3-225p^2q^2-180p^2-45pq^4+15pq^3+15pq^2+15pq+12p-117q^5-225q^4-45q^3-165q^2+12q)/120$$

(b) $S(G) = (120m^3n^2 + 160m^3n + 40m^3 + 60m^2n^3 + 360m^2n^2p + 360m^2n^2q + 360m^2n^2 - 180m^2np^2 + 360m^2np - 180m^2nq^2 + 360m^2nq + 360m^2n + 180m^2p^3 - 180m^2p^2q - 60m^2p^2 - 60m^2pq + 60m^2p - 120m^2q^2 + 60m^2q + 60m^2 + 30mn^4 + 120mn^3p + 120mn^3q + 160mn^3 + 180mn^2p^2 + 720mn^2pq + 600mn^2p + 180mn^2q^2 + 600mn^2q + 330mn^2 - 120mnp^3 - 360mnp^2q - 360mnpq^2 + 480mnpq + 480mnp - 120mnq^3 + 480mnq + 220mn + 120mp^4 + 120mp^3q + 60mp^3 - 90mp^2q^2 - 210mp^2q - 60mp^2 - 210mpq^2 + 30mpq + 60mp - 30mq^4 - 120mq^3 - 90mq^2 + 60mq + 20m - 6n^5 + 30n^4p + 30n^4q + 90n^3p^2 + 120n^3pq + 180n^3p + 30n^3q^2 + 140n^3q + 50n^3 + 120n^2p^3 + 225n^2p^2 + 180n^2pq^2 + 420n^2pq + 285n^2p - 60n^2q^3 + 75n^2q^2 + 255n^2q + 60n^2 - 180np^4 - 20np^3 - 180np^2q^2 - 150np^2q + 75np^2 - 120npq^3 - 30npq^2 + 240npq + 155np + 120nq^4 + 40nq^3 + 45nq^2 + 165nq + 16n + 72p^5 + 60p^4q - 10p^4 - 30p^3q^2 + 30p^3q - 20p^3 + 30p^2q^3 - 75p^2q^2 - 75p^2q - 50p^2 - 30pq^4 - 70pq^3 - 15pq^2 + 55pq + 8p - 78q^5 - 75q^4 - 50q^3 - 45q^2 + 8q)/60$

(c) $Gut(G) = (180m^3n^2 + 120m^3n + 20m^3 + 90m^2n^3 + 540m^2n^2p + 540m^2n^2q + 270m^2n^2 - 270m^2np^2 + 270m^2np - 270m^2nq^2 + 270m^2nq + 120m^2n + 270m^2p^3 - 270m^2p^2q - 180m^2p^2 + 90m^2pq + 30m^2p - 90m^2q^2 + 30m^2q + 45mn^4 + 180mn^3p + 180mn^3q + 120mn^3 + 270mn^2p^2 + 1080mn^2pq + 450mn^2p + 270mn^2q^2 + 450mn^2q + 165mn^2 - 180mnp^3 - 540mnp^2q - 540mnpq^2 + 360mnpq + 180mnp - 180mnq^3 + 180mnq + 90mn + 180mp^4 + 180mp^3q - 90mp^3 - 135mp^2q^2 - 225mp^2q - 150mp^2 + 45mpq^2 + 135mpq - 45mq^4 - 90mq^3 - 45mq^2 + 10m - 9n^5 + 45n^4p + 45n^4q + 135n^3p^2 + 180n^3pq + 135n^3p + 45n^3q^2 + 105n^3q + 5n^3 + 180n^2p^3 + 270n^2pq^2 + 450n^2pq + 135n^2p - 90n^2q^3 + 90n^2q^2 + 135n^2q - 270np^4 + 120np^3 - 270np^2q^2 - 180np^2q - 135np^2 - 180npq^3 - 90npq^2 + 240npq + 75np + 180nq^4 + 30nq^3 + 75nq^2 + 105nq + 4n + 108p^5 + 90p^4q - 75p^4 - 45p^3q^2 - 45p^3q - 20p^3 + 45p^2q^3 + 45p^2q^2 - 30p^2q - 75p^2 - 45pq^4 + 15pq^3 - 15pq^2 + 45pq + 2p - 117q^5 - 90q^4 - 95q^3 - 60q^2 + 2q)/30$

Example 3. Let $G = H_{q,p,m,n}$ and if $n \leq q + p$, then

(a) $W_e(G) = (180m^3n^2 + 120m^3n + 20m^3 + 90m^2n^3 + 810m^2n^2p + 270m^2n^2q - 270m^2n^2 - 270m^2np^2 - 540m^2npq + 180m^2np + 270m^2nq^2 + 360m^2nq - 180m^2n - 90m^2p^2 + 270m^2pq^2 + 90m^2pq + 30m^2p - 270m^2q^3 - 180m^2q^2 + 30m^2q - 60m^2 + 45mn^4 + 270mn^3p + 90mn^3q + 120mn^3 + 405mn^2p^2 + 1080mn^2pq - 585mn^2p + 135mn^2q^2 -$

$$\begin{aligned}
 & 675mn^2q - 75mn^2 - 180mnp^3 - 810mnp^2q + 495mnp^2 - 810mnpq^2 + 180mnpq - \\
 & 345mnp + 360mnq^3 + 765mnq^2 - 135mnq + 150mn - 45mp^4 - 90mp^3 + 405mp^2q^2 - \\
 & 45mp^2q + 75mp^2 + 180mpq^3 + 45mpq^2 + 135mpq - 60mp - 360mq^4 - 270mq^3 - 30mq^2 - \\
 & 60mq + 40m - 18n^5 + 90n^4p + 90n^4q + 90n^3p^2 + 150n^3p - 90n^3q^2 + 90n^3q - 50n^3 + \\
 & 270n^2p^3 + 270n^2p^2q - 540n^2p^2 + 540n^2pq^2 - 630n^2pq - 450n^2q^2 - 60n^2 - 315np^4 - \\
 & 180np^3q + 660np^3 - 675np^2q^2 + 315np^2q - 285np^2 - 360npq^3 + 405npq^2 - 225npq + \\
 & 180np + 270nq^4 + 660nq^3 + 30nq^2 + 240nq + 8n + 72p^5 - 225p^4 + 90p^3q^2 - 30p^3q + \\
 & 110p^3 + 360p^2q^3 - 135p^2q^2 + 165p^2q - 165p^2 + 75pq^2 + 15pq + 28p - 198q^5 - 300q^4 - \\
 & 70q^3 - 180q^2 + 28q)/120
 \end{aligned}$$

(b) $S(G) = (120m^3n^2 + 160m^3n + 40m^3 + 60m^2n^3 + 540m^2n^2p + 180m^2n^2q + 360m^2n^2 - 180m^2np^2 - 360m^2npq + 420m^2np + 180m^2nq^2 + 300m^2nq + 360m^2n - 120m^2p^2 + 180m^2pq^2 - 60m^2pq + 60m^2p - 180m^2q^3 - 60m^2q^2 + 60m^2q + 60m^2 + 30mn^4 + 180mn^3p + 60mn^3q + 160mn^3 + 270mn^2p^2 + 720mn^2pq + 750mn^2p + 90mn^2q^2 + 450mn^2q + 330mn^2 - 120mnp^3 - 540mnp^2q + 30mnp^2 - 540mnpq^2 + 240mnpq + 510mnp + 240mnq^3 + 210mnq^2 + 450mnq + 220mn - 30mp^4 - 120mp^3 + 270mp^2q^2 - 150mp^2q - 90mp^2 + 120mpq^3 - 30mpq^2 + 30mpq + 60mp - 240mq^4 - 180mq^3 - 60mq^2 + 60mq + 20m - 12n^5 + 60n^4p + 60n^4q + 60n^3p^2 + 200n^3p - 60n^3q^2 + 120n^3q + 60n^3 + 180n^2p^3 + 180n^2p^2q + 270n^2p^2 + 360n^2pq^2 + 420n^2pq + 270n^2p + 30n^2q^2 + 210n^2q + 60n^2 - 210np^4 - 120np^3q - 20np^3 - 450np^2q^2 - 210np^2q + 120np^2 - 240npq^3 - 90npq^2 + 270npq + 150np + 180nq^4 + 160nq^3 + 90nq^2 + 170nq + 12n + 48p^5 - 75p^4 + 60p^3q^2 - 40p^3q - 60p^3 + 240p^2q^3 + 45p^2q^2 - 105p^2q - 45p^2 - 15pq^2 + 55pq + 12p - 132q^5 - 130q^4 - 60q^3 - 50q^2 + 12q)/60$

(c) $Gut(G) = (180m^3n^2 + 120m^3n + 20m^3 + 90m^2n^3 + 810m^2n^2p + 270m^2n^2q + 270m^2n^2 - 270m^2np^2 - 540m^2npq + 180m^2np + 270m^2nq^2 + 360m^2nq + 120m^2n - 90m^2p^2 + 270m^2pq^2 + 90m^2pq + 30m^2p - 270m^2q^3 - 180m^2q^2 + 30m^2q + 45mn^4 + 270mn^3p + 90mn^3q + 120mn^3 + 405mn^2p^2 + 1080mn^2pq + 495mn^2p + 135mn^2q^2 + 405mn^2q + 165mn^2 - 180mnp^3 - 810mnp^2q - 45mnp^2 - 810mnpq^2 + 180mnpq + 75mnp + 360mnq^3 + 225mnq^2 + 285mnq + 90mn - 45mp^4 - 90mp^3 + 405mp^2q^2 - 45mp^2q - 45mp^2 + 180mpq^3 + 45mpq^2 + 135mpq - 360mq^4 - 270mq^3 - 150mq^2 + 10m - 18n^5 + 90n^4p + 90n^4q + 90n^3p^2 + 150n^3p - 90n^3q^2 + 90n^3q - 10n^3 + 270n^2p^3 + 270n^2p^2q + 540n^2pq^2 + 450n^2pq + 180n^2p + 90n^2q^2 + 180n^2q - 315np^4 - 180np^3q + 120np^3 - 675np^2q^2 - 225np^2q - 225np^2 - 360npq^3 - 135npq^2 + 135npq + 60np + 270nq^4 + 120nq^3 + 90nq^2 + 120nq - 2n + 72p^5 - 90p^4 + 90p^3q^2 - 30p^3q + 40p^3 + 360p^2q^3 +$

$$135p^2q^2 + 75p^2q - 60p^2 - 15pq^2 + 45pq + 8p - 198q^5 - 165q^4 - 140q^3 - 75q^2 + 8q)/30$$

Example 4. When $G = I_{2n}$,

(a) $W_e(G) = (16n^3 - 21n^2 + 14n - 3)/6$

(b) $S(G) = 2(8n^3 + 21n^2 + 19n + 3)/3$

(c) $Gut(G) = n(32n^2 + 48n + 43)/3$

Example 5. When $G = I_{2n-1}$,

(a) $W_e(G) = (n - 1)(16n^2 - 29n + 18)/6$

(b) $S(G) = 2(8n^3 + 9n^2 + 4n - 3)/3$

(c) $Gut(G) = (32n^3 + 19n - 15)/3$

Example 6. When $G = T_n$,

(a) $W_e(G) = 3n(3n^4 - 5n^2 + 2)/20$

(b) $S(G) = n(n + 1)(n + 2)(3n^2 + 6n + 1)/5$

(c) $Gut(G) = n(18n^4 + 45n^3 + 40n^2 + 15n + 2)/10$

Example 7. Let $G = P_{m,n}$ and if $m \leq n$, then

(a) $W_e(G) = -(9m^5 - 45m^4n - 90m^3n^2 - 120m^3n + 15m^3 - 180m^2n^3 + 270m^2n^2 + 75m^2n + 60m^2 - 120mn^3 + 180mn^2 - 150mn - 24m - 20n^3 + 60n^2 - 40n)/120$

(b) $S(G) = -(m + 1)(3m^4 - 15m^3n - 3m^3 - 30m^2n^2 - 65m^2n - 22m^2 - 60mn^3 - 150mn^2 - 100mn - 8m - 20n^3 - 30n^2 - 10n)/30$

(c) $Gut(G) = -(9m^5 - 45m^4n - 90m^3n^2 - 120m^3n - 5m^3 - 180m^2n^3 - 270m^2n^2 - 165m^2n - 120mn^3 - 120mn^2 - 90mn - 4m - 20n^3 - 10n)/30$

Example 8. Let $G = T_{m,n}$ and if $m \leq n$, then

(a) $W_e(G) = -(18m^5 - 45m^4n + 75m^4 + 90m^3n^2 - 240m^3n + 10m^3 - 90m^2n^3 + 225m^2n^2 - 60m^2n + 75m^2 - 60mn^3 + 105mn^2 - 105mn + 2m - 10n^3 + 30n^2 - 20n)/60$

$$(b) S(G) = -(m+1)(6m^4 - 15m^3n - m^3 + 30m^2n^2 + 35m^2n + 11m^2 - 30mn^3 - 60mn^2 - 35mn - m - 10n^3 - 15n^2 - 5n)/15$$

$$(c) Gut(G) = -(36m^5 - 90m^4n + 15m^4 + 180m^3n^2 + 60m^3n + 50m^3 - 180m^2n^3 - 90m^2n^2 - 60m^2n + 45m^2 - 120mn^3 - 90mn^2 - 90mn + 4m - 20n^3 - 10n)/30$$

Example 9. Let $G = HX(n)$. Then

$$(a) W_e(G) = 3(n-1)(246n^4 - 1049n^3 + 1611n^2 - 1044n + 240)/20$$

$$(b) S(G) = 2(3n-1)(n-1)(41n^3 - 82n^2 + 57n - 15)/5$$

$$(c) Gut(G) = (n-1)(738n^4 - 2337n^3 + 2803n^2 - 1502n + 300)/5$$

4 Concluding remark

It is hoped that the effort made in the form of extended cut method will assist in the accomplishment of exploratory as well as a good research in the computation of edge Wiener, Schultz and Gutman indices on chemical graphs fall under L_1 -graphs.

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